

Propane, 1,1,3,3-tetramethoxy-
102-52-3 | DTXSID4059255

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	0.69	0.86	0.67	0.86	0.78

Model Results

Predicted value: 1.58e-01

Global applicability domain: Inside

Local applicability domain index: 4.89e-01

Confidence level: 8.04e-01

Nearest Neighbors from the Training Set

Image not found

1,4,7,10-Tetraoxacyclododecane

Measured: -0.0400

Predicted: -0.0349

Image not found

Diethylene glycol diethyl ether

Measured: 0.39

Predicted: 3.03e-01

Image not found

1,4,7,10,13-Pentaoxacyclopentadecane

Measured: -0.480

Predicted: -0.403

Image not found

Diethoxymethane

Measured: 0.84

Predicted: 6.96e-01